

**IONIZATION POLARITY PREDICTION OF COMPOUNDS FOR
EFFICIENT MASS SPECTROMETRY**

ABSTRACT

5 A method for segregating compounds by ionization polarity for use in polarity sensitive analysis thereof comprising the steps of:

a) selecting a data base of a statistically significant group of compounds and determining the polarization, positive or negative, at which each of said compounds is ionized;

10 b) structurally analyzing the individual compounds to determine structural characteristics common to a majority of compounds which ionize at positive polarity and to determine structural characteristics common to a majority of compounds which ionize at negative polarity, as polarization determinants;

c) sequentially arranging the polarization determinants in classification trees according to percentage determination of one of said negative or positive polarization;

15 d) applying the polarization determinants in one of said classification trees in classifying a new compound for a predicted polarization of positive or negative at which said compound is ionized;

e) segregating compounds classified as ionizing at positive polarity and compounds classified as ionizing at negative polarity; and

20 f) separately analyzing the segregated compounds with the respective predicted polarities with an analysis instrument operable in different modes depending on ionization polarity.